A new class of finite difference schemes

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1. Motivation and objectives

Fluid flows in the transitional and turbulent regimes possess a wide range of length and time scales. The numerical computation of these flows therefore requires numerical methods that can accurately represent the entire, or at least a significant portion, of this range of scales. The inaccurate representation of small scales is inherent to non-spectral schemes. This can be detrimental to computations where the energy in the small scales is comparable to that in the larger scales, e.g. large-eddy simulations of high Reynolds number turbulence. The inaccurate numerical representation of the small scales in these large-eddy simulations can result in the numerical error overwhelming the contribution of the subgrid-scale model (Kravchenko & Moin 1996).

Recently, Lele (1992) introduced a family of implicit (also called compact) finite difference schemes for the spatial derivatives. The implicit schemes equate a weighted sum of the nodal derivatives to a weighted sum of the function, e.g., $f'_{i-1}+4f'_i+f'_{i+1} = 3(f_{i+1}-f_{i-1})/h$, and $f''_{i-1}+10f''_i+f''_{i+1} = 12(f_{i+1}-2f_i+f_{i-1})/h^2$. Throughout this paper, f_i and f_i^k denote the values of the function and its k^{th} derivative respectively, at the node $x = x_i$, and h denotes the uniform mesh spacing. These schemes have better small scale accuracy than explicit schemes with the same stencil width. The most popular of the implicit schemes (also called Padé schemes due to their earlier derivation from Padé approximants) appear to be the symmetric fourth and sixth order versions. There have been several recent computations of compressible flows that have used the Padé schemes. The flows computed, include transitional boundary layers, turbulent flows and flow-generated noise. The Padé schemes have been less popular in incompressible computations, presumably due to the Poisson equation generating sparse matrices when there is more than one inhomogeneous direction.

This report presents a related family of finite difference schemes for the spatial derivatives. The proposed schemes are more accurate than the standard Padé schemes, while incurring essentially the same computational cost. The objective of this report is to present these schemes as an attractive alternative to the standard Padé schemes.

This work is discussed in detail by Mahesh (1996); this report only summarizes the more prominent results.

2. Accomplishments

For the same stencil width, the standard Padé schemes are two orders higher in accuracy and have better spectral representation than the corresponding symmetric, explicit schemes. For example, $f'_{i-1} + 4f'_i + f'_{i+1} = 3(f_{i+1} - f_{i-1})/h$ is fourth order accurate, while $f_i' = (f_{i+1} - f_{i-1})/2h$ is only second order accurate. The implicit relation between the derivatives in the Padé schemes yields additional degrees of freedom that allow higher accuracy to be achieved. It is therefore to be expected, that including the second derivatives in the implicit expression would further increase the degrees of freedom, and thereby the accuracy that can be obtained. Additional motivation to solve for the first and second derivatives simultaneously, is provided by the Navier-Stokes equations requiring both derivatives of most variables. This suggests a numerical scheme of the form† :

$$a_1 f_{i-1}' + a_0 f_i' + a_2 f_{i+1}' + h(b_1 \ f_{i-1}'' + b_0 f_i'' + b_2 f_{i+1}'') = \frac{1}{h}(c_1 f_{i-2} + c_2 f_{i-1} + c_0 f_i + c_3 f_{i+1} + c_4 f_{i+2}). \tag{1}$$

Hermitian expressions involving functions and their first, and higher derivatives have been suggested in the literature (see Mahesh, 1996 for references). However, the development was not completed to a point where the resulting schemes could be used for solving partial differential equations. The objective of this paper is to develop this family of schemes, and assess their potential for computations of the Navier-Stokes equations. The schemes will be referred to as the 'coupled-derivative', or 'C-D' schemes to distinguish them from the standard Padé schemes.

2.1 The interior scheme

Simultaneous solving for f_i' and f_i'', implies that the number of unknowns is equal to $2N$. A total of $2N$ equations are therefore needed to close the system. Equation 1 may be used to derive two linearly independent equations at each node. This is done as follows. Both sides of Eq. 1 are first expanded in a Taylor series. The resulting coefficients are then matched, such that Eq. 1 maintains a certain order of accuracy. Note that Eq. 1 has eleven coefficients, of which one is arbitrary, i.e., Eq. 1 may be divided through by one of the constants, without loss of generality. A convenient choice of the normalizing constant, is either of a_0 or b_0. It will be seen that the equation obtained by setting a_0 equal to 1, is linearly independent of the equation obtained when b_0 is set equal to 1. The two equations may therefore be applied at each node, and the resulting system of $2N$ equations solved for the nodal values of the first and second derivative.

The details of this process are discussed by Mahesh (1996) and are not repeated here. Expressions ranging from second through eighth order may be obtained, depending upon the choice of coefficients. The sixth order C-D scheme has the same stencil width as the fourth order Padé scheme, while the eighth order scheme has the same stencil width as the sixth order Padé scheme. The sixth, and eighth order C-D schemes are summarized below. Note that the schemes are restricted to be symmetric. The standard Padé schemes are also presented, for completeness.

† The schemes are developed on uniform meshes. It is assumed that computations with non-uniform grids can define analytical mappings between the non-uniform grid and a corresponding uniform grid. The metrics of the mapping may then be used to relate the derivatives on the uniform grid to those on the non-uniform grid.

<u>*Sixth order C-D scheme ($c_1 = c_4 = 0$)*</u>

$$7f'_{i-1} + 16f'_i + 7f'_{i+1} + h(f''_{i-1} - f''_{i+1}) = \frac{15}{h}(f_{i+1} - f_{i-1}). \tag{2a}$$

$$9(f'_{i+1} - f'_{i-1}) - h(f''_{i-1} - 8f''_i + f''_{i+1}) = \frac{24}{h}(f_{i-1} - 2f_i + f_{i+1}). \tag{2b}$$

<u>*Eighth order C-D scheme*</u>

$$51f'_{i-1} + 108f'_i + 51f'_{i+1} + 9h(f''_{i-1} - f''_{i+1}) = \frac{107}{h}(f_{i+1} - f_{i-1}) - \frac{f_{i+2} - f_{i-2}}{h}. \tag{3a}$$

$$\begin{aligned}138(f'_{i+1} - f'_{i-1}) - h(18f''_{i-1} - 108f''_i + 18f''_{i+1}) = &-\frac{f_{i+2} + f_{i-2}}{h} \\ &+ \frac{352}{h}(f_{i+1} + f_{i-1}) - \frac{702}{h}f_i.\end{aligned} \tag{3b}$$

<u>*Standard fourth order Padé*</u>

$$f'_{i-1} + 4f'_i + f'_{i+1} = \frac{3}{h}(f_{i+1} - f_{i-1}). \tag{4a}$$

$$f''_{i-1} + 10f''_i + f''_{i+1} = \frac{12}{h^2}(f_{i-1} - 2f_i + f_{i+1}). \tag{4b}$$

<u>*Standard sixth order Padé*</u>

$$f'_{i-1} + 3f'_i + f'_{i+1} = \frac{7}{3h}(f_{i+1} - f_{i-1}) + \frac{f_{i+2} - f_{i-2}}{12h}. \tag{5a}$$

$$2f''_{i-1} + 11f''_i + 2f''_{i+1} = \frac{12}{h^2}(f_{i-1} - 2f_i + f_{i+1}) + \frac{3}{4h^2}(f_{i-2} - 2f_i + f_{i+2}). \tag{5b}$$

Fourier analysis and the concept of the 'modified wavenumber' shows that the C-D schemes are noticeably more accurate than the standard Padé schemes. Expressions for the modified wavenumber are given by Mahesh (1996). The modified wavenumbers for the first derivative are shown in Fig. 1. The C-D schemes are seen to follow the exact solution more closely than the standard Padé schemes. Recall that the sixth order C-D scheme has the same stencil width as the fourth order Padé, while the eighth order C-D scheme has the same stencil width as the sixth order Padé. In spite of its smaller stencil, the sixth order C-D scheme is seen to have lower error than the sixth order Padé. Of the different compact schemes considered by Lele (1992), the only scheme that outperforms the eighth order C-D scheme is the pentadiagonal tenth order scheme (designated 'i' by Lele). The pentadiagonal scheme, however, has a stencil of five points on the left hand side, and seven on the right.

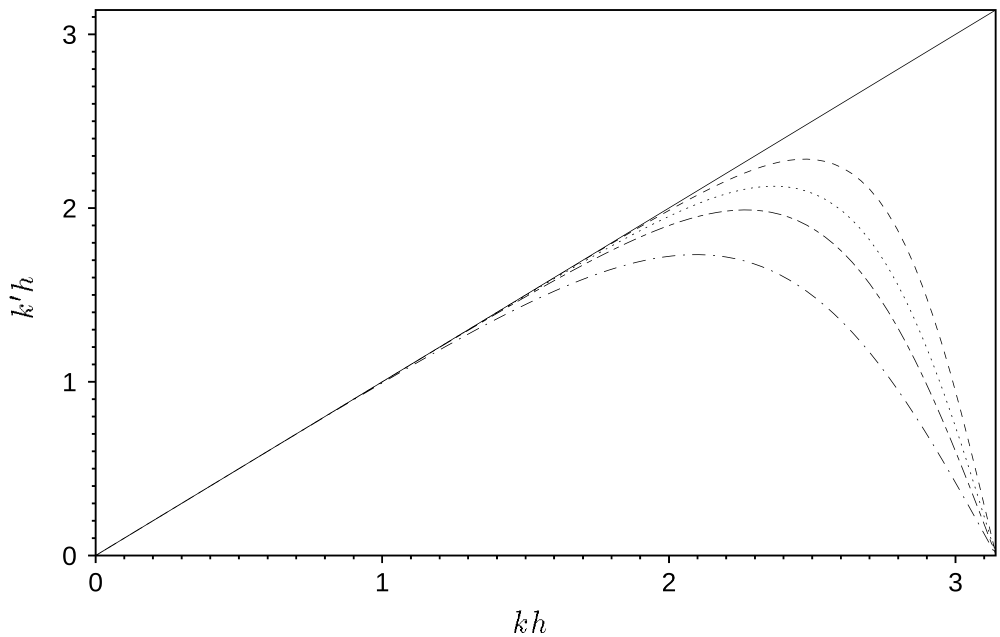

FIGURE 1. The modified wavenumber for the first derivative. The C-D schemes are compared to the standard Padé schemes. ——— (Exact), - - - - (C-D: eighth order), ········ (C-D: sixth order), —–— (Padé: sixth order), —·— (Padé: fourth order).

	$N = 4$	$N = 8$
Padé 4	4.51 %	2.3×10^{-1} %
Padé 6	0.97 %	1.2×10^{-2} %
C-D 6	0.36 %	3.1×10^{-3} %
C-D 8	0.06 %	1.1×10^{-4} %

TABLE 1. The percentage error in the first derivative, as a function of the number of points per wave (N). The C-D schemes are compared to the standard Padé schemes.

The modified wavenumber may be used to determine the error as a function of the resolution. Consider the case where $k = 1$; i.e., we have one wave of wavelength $\lambda = 2\pi$. The mesh spacing, h is given by $h = 2\pi/N = \lambda/N$. kh is therefore equal to λ/N, the reciprocal of the number of points per wavelength. Table 1 documents the percentage error in the first derivative, for resolutions of 4 and 8 points per wave. The C-D schemes are seen to represent even four delta waves with an accuracy of 0.4% and 0.06%, respectively.

Modified wavenumbers for the second derivative are shown in Fig. 2. The C-D schemes are seen to be noticeably more accurate at the higher wavenumbers. Interestingly, ${k''}^2 h^2$ for the C-D schemes is greater than the exact solution for

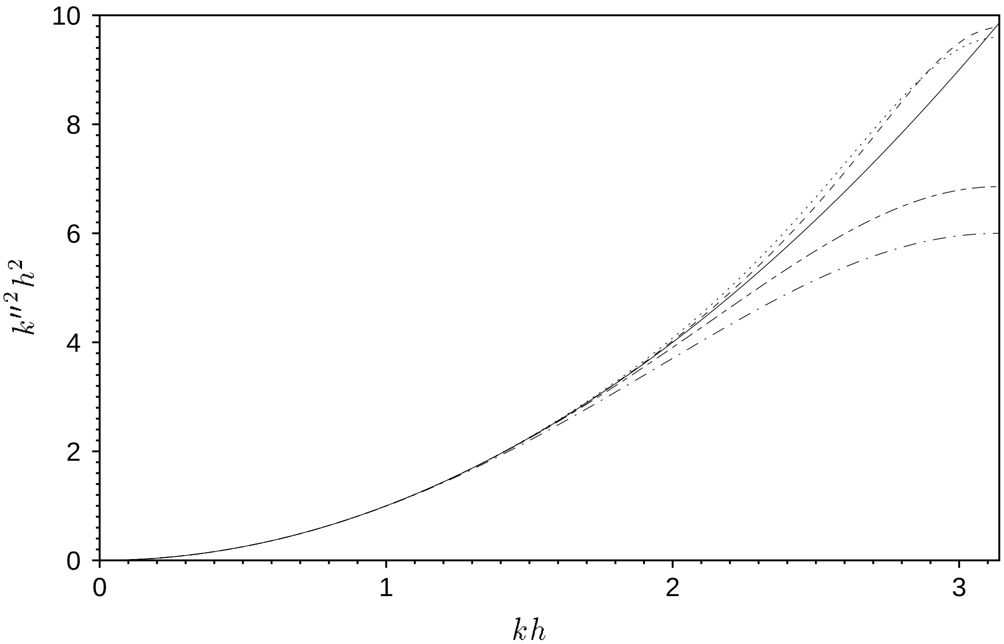

FIGURE 2. The modified wavenumber for the second derivative. The C-D schemes are compared to the standard Padé schemes. ——— (Exact), - - - - (C-D: eighth order), ········ (C-D: sixth order), —-— (Padé: sixth order), —·— (Padé: fourth order).

	$N=4$	$N=8$
Padé 4	2.73 %	1.6×10^{-1} %
Padé 6	0.52 %	7.41×10^{-3} %
C-D 6	0.44 %	6.16×10^{-3} %
C-D 8	0.09 %	2.84×10^{-4} %

TABLE 2. The percentage error in the second derivative, as a function of the number of points per wave (N). The C-D schemes are compared to the standard Padé schemes.

certain wavenumbers. This is in contrast to the standard Padé schemes, whose modified wavenumber is always less than the exact solution. Table 2 shows the percentage error in the second derivative, as a function of the resolution. As was observed for the first derivative, the sixth and eighth order C-D schemes represent even four-delta waves, to an accuracy of about 0.4% and 0.1% respectively.

2.2 The boundary schemes

Consider a spatial domain that is discretized by using N points (including those at the boundaries). Equations 2 and 3 show that the sixth order C-D scheme can be applied from $j = 2$ to $N-1$, while the eighth order scheme can be applied from $j = 3$ to $N-2$. For problems with periodic boundary conditions, the periodicity of the solution may be used to apply the same equations at the boundary nodes. However, for non-periodic problems, additional expressions are needed at the boundary nodes to close the system. These expressions are derived below.

Consider $j = 1$. The following general expression may be written for f'_1 and f''_1:

$$a_0 f'_1 + a_1 f'_2 + h(b_0 f''_1 + b_1 f''_2) = \frac{1}{h}(c_1 f_1 + c_2 f_2 + c_3 f_3 + c_4 f_4). \tag{6}$$

The corresponding equation at $j = N$ would be given by:

$$a_0 f'_N + a_1 f'_{N-1} - h(b_0 f''_N + b_1 f''_{N-1}) = -\frac{1}{h}(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3}). \tag{7}$$

The width of the stencil on the left hand side of the above equation is restricted to two. This ensures that the number of bands in the left-hand side matrix is still seven. As was done for the interior scheme, the constants in Eq. 6 may be obtained by expanding the terms in a Taylor's series, and matching expressions of the same order. Recall that we need two independent equations at each node. For the interior schemes, we saw that b_0 was equal to 0 if a_0 was equal to 1, and vice-versa. This yielded the two independent equations. This relationship between a_0 and b_0 for the interior schemes is a natural consequence of their symmetry. However for the boundary schemes, it turns out that setting a_0 to 1 does not imply that b_0 is zero. The equation obtained when $a_0 = 1$, is the same as that obtained when $b_0 = 1$. The following procedure is therefore used to obtain two independent equations. When matching the terms in the Taylor table, (a_0, b_0) is first explicitly set equal to $(1, 0)$. This yields the first equation. Next, (a_0, b_0) is set equal to $(0, 1)$, and the terms in the Taylor table are matched. This yields the second equation.

Expressions of order ranging from three to five were derived, and are outlined by Mahesh (1996). The boundary expressions were then combined with the interior scheme, and hyperbolic stability of the complete differencing scheme was examined. Numerical solutions of the one-dimensional wave equation, and eigenvalue analysis were used for this purpose. The higher order boundary closures were found to yield asymptotically unstable schemes. The following boundary closures were found to yield stable schemes, when combined with both sixth and eight order interior schemes. Note that the following equations are applied at $j = 1$. Equation 7 may be used to obtain the corresponding expressions at $j = N$. Also, recall that the sixth order interior scheme may be applied from $j = 2$ to $N-1$, while the eighth order interior scheme may be applied from $j = 3$ to $N-2$. In this report, the sixth order scheme is used at $j = 2$ and $N-1$ if the eighth order scheme is used in the interior. The stable boundary closures are as follows:

<u>(3,4) *boundary closure*</u>

The third order expression for the first derivative is combined with a fourth order expression for the second derivative.

$$f'_1 + 2f'_2 - \frac{h}{2} f''_2 = \frac{3}{h}(f_2 - f_1) \tag{8a}$$

$$-\frac{5}{2}f_2' + h(f_1'' + \frac{17}{2}f_2'') = \frac{1}{h}(\frac{34}{3}f_1 - \frac{83}{4}f_2 + 10f_3 - \frac{7}{12}f_4) \quad (8b)$$

<u>*(3, 3) boundary closure*</u>

The third order expression for the first derivative is combined with a third order expression for the second derivative.

$$f_1' + 2f_2' - \frac{h}{2}f_2'' = \frac{3}{h}(f_2 - f_1) \quad (9a)$$

$$-6f_2' + h(f_1'' + 5f_2'') = \frac{3}{h}(3f_1 - 4f_2 + f_3) \quad (9b)$$

<u>*(3, 2) boundary closure*</u>

The third order expression for the first derivative is combined with a second order expression for the second derivative.

$$f_1' + 2f_2' - \frac{h}{2}f_2'' = \frac{3}{h}(f_2 - f_1) \quad (10a)$$

$$-6f_2' + h(f_1'' + 2f_2'') = \frac{6}{h}(f_1 - f_2) \quad (10b)$$

2.3 Cost comparison

The computational cost of the C-D schemes is compared to that of the standard Padé schemes, in this section. The standard Padé schemes and the C-D schemes are both of the form,

$$\mathbf{A}\ \widetilde{\mathbf{f}} = \mathbf{B}\ \mathbf{f} \quad (11)$$

where $\mathbf{f} = [\ldots f_{i-1}, f_i, f_{i+1}, \ldots]^T$, and $\mathbf{A}$ and $\mathbf{B}$ are constant matrices that depend on the scheme. For the standard Padé schemes, the vector $\widetilde{\mathbf{f}}$ is of length N, and is either equal to $[\ldots f_{i-1}', f_i', f_{i+1}' \ldots]^T$, or $[\ldots f_{i-1}'', f_i'', f_{i+1}'' \ldots]^T$. Also, the matrix $\mathbf{A}$ is tridiagonal with a band-length of N. For the C-D schemes, $\widetilde{\mathbf{f}}$ is of length $2N$, and is equal to $[\ldots f_{i-1}', f_{i-1}'', f_i', f_i'', f_{i+1}', f_{i+1}'', \ldots]^T$. The matrix $\mathbf{A}$ now has seven bands, each of length equal to $2N$.

At first glance, it might appear as if the C-D schemes would be significantly more expensive. However, this is not the case. When the cost of computing both derivatives is estimated, the C-D schemes are seen to incur essentially the same cost as the standard Padé schemes. This is illustrated below.

In using schemes of the form given by Eq. 11, the common practice is to perform LU decomposition of the matrix $\mathbf{A}$ only once, and store the L and U matrices. Computation of the derivatives therefore involves computing the right-hand side ($\mathbf{B}\ \mathbf{f}$), followed by forward and back substitution. The operation count associated with computing the right-hand side, and solving the resulting system of equations is tabulated in Table 3. When the cost of computing both derivatives is estimated, the C-D schemes are seen to involve the same number of divides, and add/subtracts

	RHS	*LU* solve	Total
Padé 4: 1st der.	$1+1+0=2$	$2+2+1=5$	$3+3+1=7$
Padé 4: 2nd der.	$2+2+0=4$	$2+2+1=5$	$4+4+1=9$
Padé 6: 1st der.	$2+3+0=5$	$2+2+1=5$	$4+5+1=10$
Padé 6: 2nd der.	$4+5+0=9$	$2+2+1=5$	$6+7+1=14$
Padé 4: both ders.	$3+3+0=6$	$4+4+2=10$	$7+7+2=16$
Padé 6: both ders.	$6+8+0=14$	$4+4+2=10$	$10+12+2=24$
C-D 6	$3+3+0=6$	$12+4+2=18$	$15+7+2=24$
C-D 8	$3+7+0=10$	$12+4+2=18$	$15+11+2=28$

TABLE 3. The operation count per node to compute the first and second derivative. The entries are of the form, 'number of multiplies + adds/subtracts + divides = total'. The overall cost is obtained by multiplying the entries by the total number of points, N.

as the standard Padé schemes with the same stencil width. The only increase in the number of operations involves the number of multiplies: the eighth order scheme has 1.5 times the number of multiplies as the sixth order Padé, while the sixth order scheme has twice the number of multiplies as the fourth order Padé. A numerical evaluation of the derivatives (Mahesh, 1996) shows this increase in the number of multiplies is not very significant.

3. Conclusions

A new class of finite difference schemes for the first and second derivatives of smooth functions was proposed. The schemes are Hermitian, symmetric, and solve for the first and second derivatives simultaneously. They are two orders higher in accuracy than the standard Padé schemes with the same stencil width, and have noticeably better spectral representation. The computational cost of computing both derivatives is essentially the same as the Padé schemes. The proposed schemes are attractive alternatives to the Padé schemes, for Navier-Stokes computations.

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REFERENCES

KRAVCHENKO, A. G. & MOIN, P. 1996 On the effect of numerical errors in large eddy simulations of turbulent flows. *CTR Manuscript 160,* To appear in *J. Comp. Phys.*

LELE, S. K. 1992 Compact finite difference schemes with spectral-like resolution. *J. Comp. Phys.* **103,** 16-42.

MAHESH, K. 1996 A family of finite difference schemes with good spectral resolution. *CTR Manuscript 162,* Submitted to *J. Comp. Phys.*